ON A VARIATIONAL PRINCIPLE IN THE STATISTICAL MANY-BODY PROBLEM

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Abstract

Full Text

PHYSICS

I. A. Kvasnikov and V. V. Tolmachev

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In the work ([1]), N. N. Bogolyubov, considering a dynamical system of Fermi particles with pair interaction, proposed a new approximate variational method in the many-body problem, which, as he showed, is a generalization of the well-known Fock method. It appears interesting to generalize the method ([1]) and to formulate a statistical variational principle suitable for determining thermodynamic quantities both at zero and at nonzero temperatures, especially since the statistical treatment of the many-body problem is the most fruitful. In the present note we shall try to carry out this program.

Let us consider a system of Fermi particles with Hamiltonian

$$H = \sum \{T(f, f') - \lambda \delta_{f,f'}\} a_f^+ a_{f'} + \frac{1}{2} \sum J(f_1, f_2; f_2', f_1') a_{f_1}^+ a_{f_2}^+ a_{f_2'} a_{f_1'}, \tag{1}$$

where λ is the chemical potential; f is the set of indices determining the state of one particle; as regards J, without loss of generality one may assume that

$$J(f_1, f_2; f_2', f_1') = -J(f_1, f_2; f_1', f_2') = -J(f_2, f_1; f_2', f_1').$$

We pass from the operators a, by means of a canonical transformation, to new Fermi amplitudes α:

$$a_f = \sum_\nu (u_{f\nu} \alpha_\nu + v_{f\nu} \alpha_\nu^+), \tag{2}$$

with

$$\xi(f, f') \equiv \sum_\nu (u_{f\nu} u_{f'\nu}^* + v_{f\nu} v_{f'\nu}^*) = \delta_{f,f'},$$

$$\eta(f, f') \equiv \sum_\nu (u_{f\nu} v_{f'\nu} + v_{f\nu} u_{f'\nu}) = 0. \tag{3}$$

The coefficient functions u, v entering into this transformation will in what follows play the role of variational parameters. At the same time, in order to construct the statistical variational principle, in contrast to the variational principle of the work ([1]), it is no longer sufficient for us to specify only one "trial" vacuum state C_0:

$$\alpha_\nu C_0 = 0, \tag{4}$$

but it is also necessary to know the "trial" excitations. This is achieved by the following choice of the zero Hamiltonian:

$$H = U + H_0 + H_1, \tag{5}$$

where

$$U = \langle C_0^* H C_0 \rangle, \qquad H_0 = \sum_\mu E_\mu \alpha_\mu^+ \alpha_\mu, \tag{6}$$

where E_μ is the difference between the energies of the excited state $\alpha_\mu^+ C_0$ and the vacuum state C_0:

$$E_\mu = \langle C_0^* \alpha_\mu H \alpha_\mu^+ C_0 \rangle - \langle C_0^* H C_0 \rangle = \langle C_0^* \alpha_\mu H \alpha_\mu^+ C_0 \rangle_{\text{conn}}. \tag{7}$$

For the separation of the Hamiltonian adopted in (5) we now apply the variational theorem of N. N. Bogolyubov, which gives an estimate of the upper bound of the thermodynamic potential:

$$\Omega = -\theta \ln \operatorname{Sp} e^{-H/\theta}. \tag{8}$$

According to this theorem

$$\Omega \leqslant -\theta \ln \operatorname{Sp} e^{-H_0/\theta} + \frac{\operatorname{Sp}\{(U + H_1) e^{-H_0/\theta}\}}{\operatorname{Sp} e^{-H_0/\theta}}. \tag{9}$$

Expanding the right-hand side of inequality (9), we obtain for it:

$$\Omega = -\theta \sum_\mu \ln(1 + e^{-E_\mu/\theta}) + U + \sum J(f_1, f_2; f_2', f_1') \{ u^*_{f_1\nu_1} u^*_{f_2\nu_2} u_{f_2'\nu_2'} u_{f_1'\nu_1'}$$
$$+ 2u^*_{f_1\nu_1} v^*_{f_2\nu_1} v_{f_2'\nu_2'} u_{f_1'\nu_2'} + 2u^*_{f_1\nu_1} v^*_{f_2\nu_2} u_{f_2'\nu_2'} v_{f_1'\nu_2'} + v^*_{f_1\nu_1} v^*_{f_2\nu_2} v_{f_2'\nu_1'} v_{f_1'\nu_2'} \} \bar{n}_{\nu_1} \bar{n}_{\nu_2}, \tag{10}$$

where

$$\bar{n}_\nu = \frac{1}{1+e^{E_\nu/\theta}},$$

$$U = \frac{1}{2}\sum J(f_1, f_2; f_2', f_1')\{2v^*_{f_1\nu_1}v^*_{f_2\nu_2}v_{f_2'\nu_2'}v_{f_1'\nu_1'} - v^*_{f_1\nu_1}u^*_{f_2\nu_2}u_{f_2'\nu_2'}v_{f_1'\nu_2'}\},$$

$$E_\mu = \sum\{T(f,f') - \lambda\delta_{ff'}\}(u^*_{f\mu}u_{f'\mu} - v^*_{f\mu}v_{f'\mu}) + \tag{11}$$

$$+\sum J(f_1, f_2; f_2', f_1')\sum_\nu\{2u^*_{f_1\mu}u^*_{f_2\nu}v_{f_2'\nu}v_{f_1'\mu} + u^*_{f_1\mu}v^*_{f_2\nu}u_{f_2'\mu}v_{f_1'\nu}$$
$$+v^*_{f_1\mu}u^*_{f_2\nu}v_{f_2'\mu}u_{f_1'\mu} - 2v^*_{f_1\mu}u^*_{f_2\nu}v_{f_2'\nu}v_{f_1'\mu}\}.$$

The variational parameters u, v are now determined from the condition that expression (10) be a minimum, taking into account the additional conditions (3):

$$\delta\widetilde{\Omega}(u,v) = 0, \tag{12}$$

$$\widetilde{\Omega}(u,v) + \Omega(u,v) = \sum_{f,f'}\{\lambda(f,f')\xi(f,f') + \mu(f,f')\eta(f,f') + \mu^*(f,f')\eta^*(f,f')\},$$

where $\lambda(f,f')$ and $\mu(f,f')$ are Euler multipliers. The u, v determined in this way are substituted into (9), and the expression obtained is identified with the potential (8). We note that at $\theta = 0$ the method set forth goes over into the variational principle of the work (1).

The method considered, in essence, had already been implicitly applied earlier by one of the authors ([4]) to the model Hamiltonian of the theory of superconductivity. In doing so it turned out that it leads to the asymptotically exact solution of the problem obtained in ([3]). Thus, the formulated variational principle gives an exact solution for a whole class of problems with a quartic Hamiltonian.

As another example, let us consider in more detail the application of the static variational method to a system whose Hamiltonian takes into account only the interactions of pairs of particles with opposite momenta:

$$H = \sum_{(k\sigma)}\{E(k) - \lambda\}a^+_{k\sigma}a_{k\sigma} +$$

$$+\frac{1}{2V}\sum_{(kk'\sigma_1\sigma_2\sigma_2'\sigma_1')} J(k,k' \mid \sigma_1,\sigma_2,\sigma_2',\sigma_1')a^+_{k\sigma_1}a^+_{-k\sigma_2}a_{-k'\sigma_2'}a_{k'\sigma_1'}, \tag{13}$$

where V is the volume of the system; σ is a discrete index characterizing the state of the particle in addition to the momentum. For the case $\theta = 0$ this example was studied in detail in the work ([2]), in which a criterion was established for the appearance of superfluidity of nuclear matter. Assuming that nuclear matter is superfluid, let us now determine, with the aid of the statistical variational principle formulated above, the critical temperature at which this phenomenon sets in. Using the notation introduced in ([2]), we shall characterize the pair $(\mathbf{k}, -\mathbf{k})$ by the index q, and the momentum $\mathbf{k}$ by two indices (q, ρ), where $\rho = \pm 1$. Then, putting $s = (\sigma, \rho)$, we have:

$$H = \sum_{(qs)} \{E(q) - \lambda\} a^+_{qs} a_{qs} +$$

$$+ \frac{1}{2V} \sum_{(qq' s_1 s_2 s'_2 s'_1)} I(q, q' \mid s_1, s_2, s'_2, s'_1)\, a^+_{qs_1} a^+_{qs_2} a_{q' s'_2} a_{q' s'_1}. \tag{14}$$

Let us perform a canonical transformation of the Fermi operators:

$$a_{qs} = \sum_{s'} \{u(q, s, s')\alpha_{qs'} + v(q, s, s')\alpha^+_{qs'}\},$$

$$\xi(q, s, s') \equiv \sum_{s''} \{u^*(q, s, s'')u(q, s', s'') + v^*(q, s, s'')v(q, s', s'')\} = \delta_{s,s'}, \tag{15}$$

$$\eta(q, s, s') \equiv \sum_{s''} \{u(q, s, s'')v(q, s', s'') + v(q, s, s'')u(q, s', s'')\} = 0.$$

Then, using relations (5)–(9) for the transformed Hamiltonian, we obtain

$$\Omega = -\theta \sum_{(qs)} \ln\left(2 \operatorname{ch} \frac{E_{qs}}{2\theta}\right) + \frac{1}{2} \sum_{(qss')} (E(q) - \lambda) +$$

$$+ \sum_{(qs)} \frac{1}{2} \operatorname{th} \frac{E_{qs}}{2\theta} \cdot \frac{1}{V} \sum_{(q' s_1 s_2 s'_2 s'_1)} \{I(q, q' \mid s_1, s_2, s'_2, s'_1) u^*(q, s_1, s) v^*(q, s_2, s) \times$$

$$\times \sum_{(s'')} v(q', s'_1, s'') u(q', s'_2, s'') + \text{conj.}\} -$$

$$- \frac{1}{2V} \sum_{(qq' s_1 s_2 s'_2 s'_1\, ss'')} I(q, q' \mid s_1, s_2, s'_2, s'_1) u^*(q, s_1, s') v^*(q, s_2, s') v(q', s'_1, s'') u(q', s'_2, s'') \times$$

$$\times \operatorname{th} \frac{E_{qs'}}{2\theta} \cdot \operatorname{th} \frac{E_{q' s''}}{2\theta}, \tag{16}$$

$$E_{qs} = (E(q)-\lambda)\sum_{(s')}\{u^*(q,s',s)u(q,s',s) - v(q,s',s)v^*(q,s',s)\}+$$
$$+\frac{1}{V}\sum_{(q's_1s_2s_2's_1')}\{I(q,q' \mid s_1,s_2,s_2',s_1')u^*(q,s_1,s)v^*(q,s_2,s)\times$$
$$\times\sum_{(s'')}u(q',s_2',s'')v(q',s_1',s'') + \text{conj.}\}. \tag{17}$$

Equating to zero the first variation of expression (16) with the additional conditions (15), and regarding the variations $\delta u, \delta u^*, \delta v, \delta v^*$ as independent, one can obtain equations for u, v, whose solutions, when substituted into (16), determine the desired thermodynamic potential. We note that these

the equations admit a trivial solution corresponding to the "normal" state:

$$u(q,s,s') = \theta_G(q)\delta_{s,s'}, \qquad v(q,s,s') = \theta_F(q)\delta_{s,s'},$$

$$\mu(q,s,s') = 0, \qquad \lambda(q,s,s') = |E(q)-\lambda|\,\frac{1}{2}\,\text{th}\,\frac{E_{qs}}{2\theta}\,\delta_{s,s'}, \tag{18}$$

where $\theta_F(q)$ is equal to unity inside the Fermi sphere and to zero outside it, $\theta_G(q) = 1-\theta_F(q)$. It is easy to see that for the solution (18)

$$E_{qs} = |E(q)-\lambda|.$$

Let us now examine the question of the stability of the "normal" state of the system by constructing the expression for the second variation $\tilde{\Omega}^{(n)}$ for the solution (18). We find:

$$2\delta^2\tilde{\Omega}^{(n)}(u,v) = \sum_{(qss')} 2|E(q)-\lambda|\,\text{cth}\,\frac{|E(q)-\lambda|}{2\theta}\,\Psi^*(q,s',s)\Psi(q,s',s)+$$
$$+\frac{1}{V}\sum_{(qq's_1s_2s_2's_1')} I(q,q'|s_1,s_2,s_2',s_1')\Psi^*(q,s_1,s_2)\Psi(q',s_1',s_2'), \tag{19}$$

where

$$\Psi^*(q,s,s') = \{\theta_F(q)\delta u^*(q,s,s') + \theta_G(q)\delta v^*(q,s',s)\}\,\text{th}\,\frac{|E(q)-\lambda|}{2\theta}.$$

We see that a stable "normal" state, corresponding to $\delta^2\tilde{\Omega} > 0$, will occur if and only if all eigenvalues of the equation

$$2|E(q)-\lambda|\,\mathrm{cth}\,\frac{|E(q)-\lambda|}{2\theta}\Psi(q,s_1,s_2)+$$

$$+\frac{1}{V}\sum_{(q's_2's_1')}I(q,q'|s_1,s_2,s_2',s_1')\Psi(q',s_1',s_2')=E\Psi(q,s_1,s_2) \qquad (20)$$

are positive. In the opposite case, when negative eigenvalues exist, the normal phase is unstable and there arises a minimum value $\Omega^{(s)}(u,v)$ of another type, determined by a nontrivial solution of the equations for u and v. At $\theta=0$, equation (20) goes over into the criterion, obtained in paper [(2)], for the existence of superfluidity of nuclear matter. Assuming that this criterion is satisfied at $\theta=0$, by means of (20) we obtain the equation for the critical temperature θ_0 at which the superfluid phase disappears:

$$2|E(q)-\lambda|\,\mathrm{cth}\,\frac{|E(q)-\lambda|}{2\theta}\Psi(q,s_1,s_2)+$$

$$+\frac{1}{V}\sum_{(q's_2's_1')}I(q,q'|s_1,s_2,s_2',s_1')\Psi(q',s_1',s_2')=0.$$

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Note: Figure translations are in progress. See original paper for figures.